SCIENCE AND TECHNOLOGY FOR ENERGY AND NATIONAL SECURITY

Celebrating 25 Years 1979-2004

CRF NEWS

COMBUSTION RESEARCH FACILITY

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CRF Engine Researchers Build Scientific Knowledge Base for Development Engineers

Patrick Flynn

This is the third in a series of articles commemorating the CRF's 25th anniversary. Patrick Flynn, former Vice President of Research at Cummins, Inc., highlights significant contributions of the CRF's engine combustion research group.

Historically, engine development was done empirically by development engineers employed by engine manufacturers. With evolving pollution control requirements, this development process has become more challenging. Increasingly stringent emissions standards are reducing the design space that allows fuel oxidation suitable for emission-controlled engine combustion.

The CRF offers a unique contribution to the scientific side of engine development. Since engine power production requires the management of combustion processes to convert chemical energy to heat and subsequently to mechanical work in an expansion process, managing the combustion process is key to all engine developers. The CRF's contributions to combustion and fluid mechanics diagnostics and to the modeling of chemical kinetics with the CHEMKIN™ programs have laid the groundwork for effectively handling these difficult tasks. The suite

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Sandia National Laboratories

Improving Laser Diagnostics

Picosecond Lasers Provide Interference-Free Two-Dimensional Measurements of Atomic Oxygen in Flames

Quantitative measurements of atomic oxygen in flames are important for studying pollutant formation from combustion. Such measurements provide insight into the effects of turbulent flow on NO production, in which the atomic oxygen radical plays a significant role. However, accurate O-atom measurements have been hampered by the shortcomings of existing laser diagnostic methods, particularly by photolytic interference generated by the laser pulses themselves.

Using picosecond (ps) lasers to eliminate this interference, Jonathan Frank and Tom Settersten have recently demonstrated two-dimensional interference-free imaging of atomic oxygen, which is important for studying the effects of flow transients on thermal NO formation.

Building on results of a previous collaboration between CRF researchers and visiting researcher Andreas Dreizler (Technical University of Darmstadt), Frank and Settersten have also shown that the dominant source of this photolytic interference in hydrocarbon flames is the photodissociation of thermally excited CO_2, not O_2, as previously thought. Their work on interference-free two-photon laser-induced fluorescence (LIF) imaging of atomic oxygen appears in the April 20 issue of *Applied Optics* and will be presented at the 30th International Symposium on Combustion.

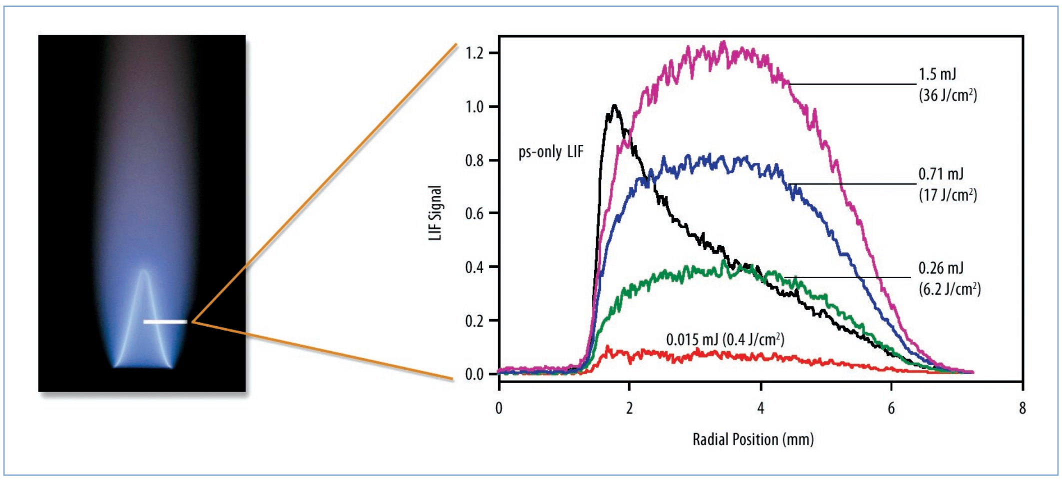

Figure 1. Radial profiles of O-atom LIF from photolytically produced O atoms in a lean (ϕ=0.70) premixed $CH_4/O_2/N_2$ flame at four ns-laser energies. Measurements were performed with a ns photolysis laser and a ps probe laser. For comparison, a LIF profile measured with only the ps laser is displayed on the same scale.

Nanosecond vs. Picosecond Lasers

Previous attempts at O-atom LIF measurements used nanosecond (ns) pulsed lasers for excitation. However, ns lasers generate significant amounts of atomic oxygen that interfere with

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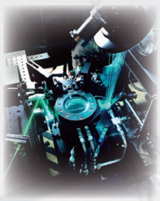
COMBUSTION RESEARCH FACILITY

25 Engine Combustion Research MILESTONES AT THE CRF

1976 Sandia engine researchers form a working group with General Motors Research, Los Alamos Scientific Laboratory, and Princeton University to improve understanding of in-cylinder processes in direct-injection stratified-charge (DISC) engines. Other working groups on dilute homogeneous-charge spark-ignition engines, knock, and diesel engines soon follow. Led by the CRF, these groups foster collaboration among industry, universities, and national laboratories, a theme central to CRF engine research in ensuing years.

1979 Optically accessible, side-valve DISC engines are designed and built at the CRF to enable time- and space-resolved in situ measurements of fuel-air ratio, velocity, and turbulence by laser techniques.

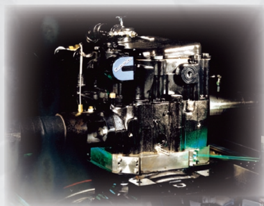
1980 CRF opens. The engines group occupies four labs, three with side-valve optical engines dedicated to laser velocimetry, Raman scattering, and flame structure imaging, and the other with a constant-volume combustion vessel for flame-propagation investigations.

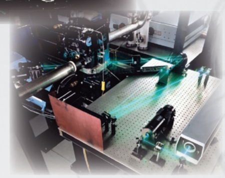


1982 One-dimensional imaging of Rayleigh-scattered light is used to measure the instantaneous thickness of a propagating turbulent flame, showing that a flame in a spark-ignition (SI) engine is not a thick flame but a thin, wrinkled, laminar flame.

Four-day short course, "Optical Diagnostics in Internal Combustion Engines," is hosted by the CRF for university, industry, and government research lab participants.

1986-1989 CRF's first optically accessible, single-cylinder research engine with a realistic head is assembled, based on a Cummins heavy-duty, N14-series diesel. Early investigations focus on in-cylinder gas flow.

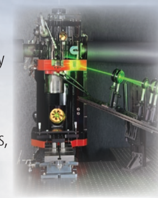




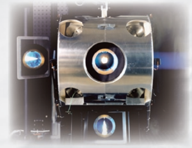
1987 CARS is used to make the first measurements of cylinder wall thermal boundary layers, which control heat losses in an engine combustion chamber.

1989 Fiber-optic spark plug probe is developed for studying early flame kernel development. Barrack Laboratories commercializes the probe in 1989.

1993 First drop-down cylinder liner is introduced on the Cummins heavy-duty diesel engine. The technology allows for rapid cleaning of combustion chamber windows, dramatically improving research throughput. Concept is later incorporated into all CRF optical engines, as well as engines at many other research institutions.



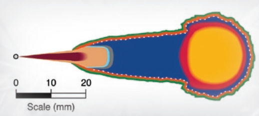
1994 New high-pressure combustion vessel for investigating diesel combustion processes is introduced. Complete optical access coupled with the capability to simulate a large range of engine thermodynamic conditions make the vessel unique in the world.



mid -1990s CRF engine group replaces side-valve research engines with production-like, spark-ignited engine configurations. In addition, two new optical diesel engines with realistic in-cylinder geometries become operational: a heavy-duty diesel based on a Caterpillar C-10 and a high-speed, direct-injection (HSDI) automotive diesel. The production-like engine configurations help ensure applicability of data to real-world engines.

1996 New diesel fuel-jet scaling law is developed that provides a comprehensive picture of engine and injector effects on fuel jet development.

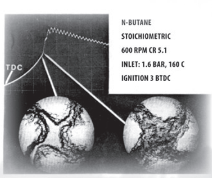
1997 CRF researchers develop a new conceptual picture of heavy-duty diesel combustion, culminating nearly a decade of research. New description shows that fuel-air mixing and soot formation in a diesel fuel jet occurs differently than previously thought and that combustion is a two-stage process involving a fuel-rich reaction and a diffusion flame. This understanding spurs new directions in diesel research worldwide.



1976 1980 1985 1990

1983 CRF develops and demonstrates laser velocimetry techniques for measuring cycle-resolved turbulence intensities, turbulence length scales, and burned and unburned flow velocities in engines.

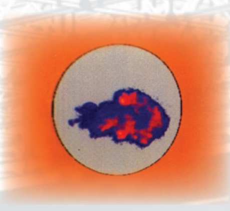
1984-1985 Measurements of temperature with coherent anti-Stokes Raman scattering (CARS) coupled with measurements of OH radical, formaldehyde, and stable species concentrations in the end gases prior to "knock" in an SI engine contribute to new understanding of the chemistry of knock, developed in collaboration with an industry/national lab team.



1985 CRF researchers develop new insight into the autoignition characteristics of future diesel fuels and the shortcomings of the current diesel fuel ignition-quality rating procedure.

1986-1988 CRF researchers demonstrate feasibility of using the RAPRENOx (Rapid Reduction of Nitrogen Oxides) process to remove NO_x from diesel exhaust and establish its temperature operating domain. NO_x reductions from 440 ppm to 5 ppm are shown. RAPRENOx wins an IR100 award in 1987.

1991 CRF and visiting Cummins Engine Company researchers are the first to develop and use laser-induced incandescence as a soot-imaging tool. Initial soot distribution studies lay the groundwork for later development of a new description of diesel engine combustion (see 1997).



1992 Ionization-probe incorporated in a printed-circuit-board head gasket for measuring flame development in spark-ignition engines wins R&D 100 award.

1998 Line-imaging of Raman scattered light is applied to fully characterize instantaneous local fuel/air ratio and exhaust gas recirculation (EGR) fraction simultaneously at multiple locations in an engine.

Single-shot planar laser-induced fluorescence (PLIF) images of NO (the source of NO_x emissions) are obtained in a heavy-duty diesel engine. The images show where and when NO is formed, providing important insight into how NO formation is related to the overall diesel combustion process.

1999 Diesel fuel jet scaling law is extended to include the penetration and vaporization of liquid-phase fuel. This scaling law provides new understanding of rate controlling processes in diesel fuel jets and guidance on avoiding liquid fuel impingement on cylinder walls, a source of poor combustion and emissions.

CRF research leads to new infrared laser-extinction technique for measuring real-time distributions of EGR in the intake manifold. Diagnostic is demonstrated at Ford and Navistar and influences the design of production engines.

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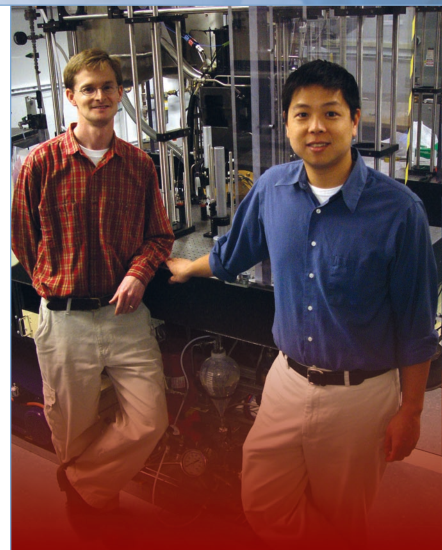
Sandia Named Center of Excellence to Advance Metal Hydride Materials Development for Hydrogen Storage

The Department of Energy has named Sandia a Center of Excellence for research in metal hydrides hydrogen storage. The center is one of three Centers of Excellence announced in April by Secretary of Energy Spencer Abraham to support President Bush's Hydrogen Fuel Initiative. Each center will take a different approach in addressing the major technical barrier to onboard hydrogen storage: storing enough hydrogen to enable a 300+-mile driving range without impacting cargo or passenger space.

Les Shephard (left), Sandia vice president of energy, information, and infrastructure surety, speaks at the April 27 event at the National Renewable Energy Laboratory announcing three Centers of Excellence for exploratory research in hydrogen storage. At right is Energy Secretary Spencer Abraham.

Selected through a merit-reviewed, competitive process, Sandia will lead a team consisting of four other national laboratories, eight universities, and three companies. Sandia researchers have developed a new class of hydrides called complex metal hydrides, which operate at pressures and temperatures that are close to ambient conditions.

Sandian Jim Wang will serve as director of the Metal Hydrides Center of Excellence (MHCoE); CRF manager Jay Keller oversees Sandia's hydrogen program. Sandia's MHCoE partners are Brookhaven National Laboratory; Oak Ridge National Laboratory; Jet Propulsion Laboratory; National Institute of Standards and Technology; University of Hawaii; University of Pittsburgh; Carnegie Mellon University; University of Nevada, Reno; University of Illinois, Urbana-Champaign; University of Utah; California Institute of Technology; Stanford University; General Electric Global Research; HRL Laboratories; and Intematix.



A. S. (Ed) Cheng (right), an assistant professor in the Department of Mechanical Engineering at California State University, Sacramento, and Sandian Chuck Mueller (left) recently completed experiments looking at why direct-injection diesel engines tend to produce higher NO_x emissions when fueled with biodiesel (fatty acid methyl esters) than with traditional diesel fuel. The "biodiesel NO_x problem" has been a barrier to the broader use of this otherwise attractive renewable fuel. Experiments were conducted in an optically accessible, single-cylinder version of a Caterpillar C-10 heavy-duty engine. Cheng, whose work with Mueller and postdoc Ansis Upatnieks began in May 2003, will continue working at the CRF as a visiting researcher.

Kliner and Co-Inventors Receive Patent Award

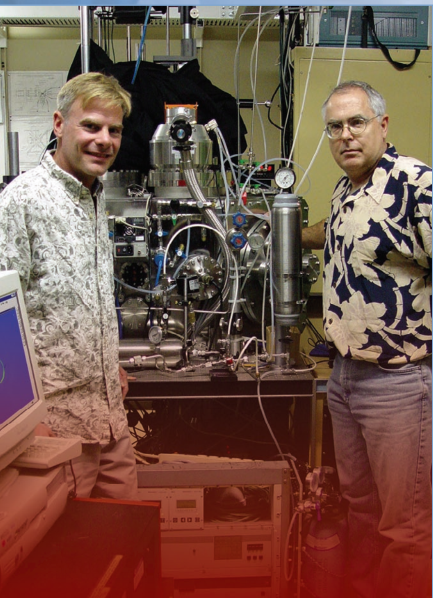
Sandian Dahv Kliner and two co-inventors at the Naval Research Laboratory (NRL) have received NRL's 2003 Edison Patent Award, which recognizes the most significant patent of the year. Their patent entitled, "Helical Fiber Amplifier," covers a coiling technique that allows at least a 100-fold increase in the power and pulse energy of fiber lasers with no loss in beam quality or efficiency. Sandia, NRL, and three separate companies are negotiating licenses to commercialize the technology.

Blevins to Manage NSF Combustion Program

Sandian Linda Blevins is taking a one- to two-year leave of absence to serve as the Program Director for Combustion and Plasma Systems at the National Science Foundation (NSF) in Arlington, Va. She will manage a program that funds basic research in U.S. universities. Her position involves overseeing the proposal process, making funding recommendations, planning future research, building multi-agency programs, sponsoring workshops, and monitoring grants.

DOE Office of Science Officials Visit CRF

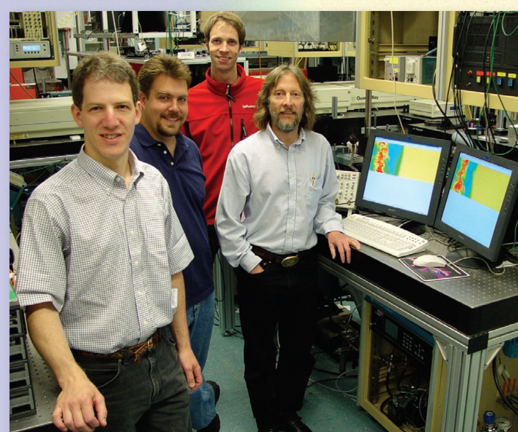
U.S. Department of Energy Office of Science Director Ray Orbach and three other DOE officials spent much of May 15 at the CRF, touring labs and learning about the CRF's research and capabilities. In the photograph above, John Dec (far right) explains the CRF's work on homogeneous charge compression ignition engines to (left to right) Michael Strayer of the Office of Advanced Strategic Computing Research, Chief of Staff Jeffrey Salmon, Orbach, Principal Deputy Director James Decker, and Sandia Vice President Pace VanDevender. Below, Sandian Craig Taatjes discusses combustion chemistry mechanisms with Salmon, VanDevender, and Orbach.



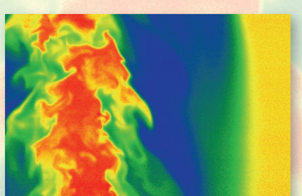
Postdoc Michael Elioff left the CRF in June after accepting a faculty position with Mississippi University for Women. He had worked with CRF senior scientist David Chandler since September 2001 using velocity-mapped ion imaging to determine inelastic scattering differential cross-sections and, more recently, colliding molecular beams for sub-kelvin translational cooling of molecules.

Matthew Reagan (right), who has been working in the CRF's Diagnostics and Reacting Flows Department, is leaving this summer to take a scientist position at Lawrence Berkeley National Laboratory. Reagan has been working with fellow Sandian Habib Najm (left), in collaboration with Johns Hopkins University, on uncertainty quantification in computations of reacting flow.

Yale Collaborators Use Advanced Imaging Laboratory



Professor Marshall Long (right) and Ph.D. student Sebastian Kaiser (middle right) from Yale University visited the CRF in May and June as part of an ongoing collaboration with Jonathan Frank (far left) and Ron Sigurdsson (middle left) in the Advanced Imaging Laboratory. Long is chair of the Department of Mechanical Engineering and director of the Center for Laser Diagnostics at Yale.



The researchers conducted multiscalar imaging experiments to determine 2-D distributions of reaction rate, mixture fraction, scalar dissipation, and temperature in turbulent jet flames. The results will be coupled with models of turbulent nonpremixed combustion and will be available through the International Workshop on Measurement and Computation of Turbulent Nonpremixed Flames **(www.ca.sandia.gov/TNF)**.

A Legacy of Industry Recognition

Over the past nearly 25 years, researchers in the CRF's engine group have received numerous honors from the Society of Automotive Engineers (SAE), the leading international professional association for the automotive and heavy-duty transportation industry, with about 84,000 members worldwide. Major SAE awards to CRF researchers include:

- SAE Fellow (3 honorees), an honor bestowed on less than 500 SAE members
- Horning Awards (4), one of the highest honors given by the SAE annually for engine/fuels related research
- Arch T. Colwell Merit Award (4) for an outstanding contribution to the SAE literature
- Forrest R. McFarland Award (2) for service to SAE
- Lloyd L. Withrow Distinguished Speaker Award (2)
- 14 individual awards for excellence in oral presentation

The awards and honors serve to recognize the significant contributions of the CRF to a better understanding of the science behind engine combustion and the emissions process, which is needed by engine manufacturers to enable the design of ever-more efficient, emission-compliant engines.

Engine Research

(Continued from page 1)

of CHEMKIN analysis tools allows the incorporation of fundamental chemical kinetics data into analytical approaches for engine combustion problems. Such approaches will become increasingly important to engine designers as the viable combustion design space continues to be further constrained by emission controls.

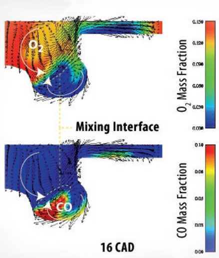
Early work at the CRF developed the most advanced laser diagnostic tools for combustion analysis. These laser diagnostics were used to delineate the fluid mechanic and chemical interactions in premixed flames. A key early discovery was the thin, rumpled nature of turbulent premixed flames. Flame propagation, knock, and homogeneous charge ignition can all be modeled in detail with tools developed by CRF researchers. These tools have recently been incorporated in a variety of analytical procedures, such as 3D viscous fluid mechanics programs, now used by engine company engineers.

In the mid-1990s, detailed diagnostic investigations into the structure and kinetics of diesel combustion revealed a surprising two-stage combustion process. At the time, this two-stage process was a new revelation to diesel engine development engineers. Later analysis with CHEMKIN portrayed the chemical kinetic constraints on fuel jet combustion processes, and how these constraints caused the observed diesel flame structures. This knowledge, along with the basic chemical kinetics drivers, continues to be detailed in the ongoing fuel jet-based combustion research.

This arsenal of diagnostic tools, models, and detailed chemical kinetic knowledge provides mechanisms, especially as they are made available to development engineers, for continuing progress in the management of combustion processes to produce very low emissions. As combustion processes continue to be modified to limit gaseous and particulate emissions, it will become necessary to understand the processes in more detail and to be able to perform analytical and empirical experiments exploring the limits of the combustion design space. I feel that these tools provided by the CRF will play an ever-increasing role in engine design evolution.

1995 **2000** **2004**

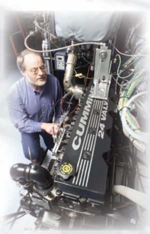
01 CRF researchers show that the amount of fuel/air mixing upstream of the flame lift-off is an important tor controlling the amount of soot formed in a diesel fuel providing new derstanding of cesses controlling t formation in sel engines.

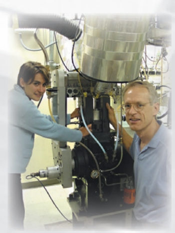


f Wisconsin researchers discover a previously unknown in HSDI automotive diesels. The knowledge contributes to -cylinder turbulence in HSDI engines to reduce emissions.

on between the CRF and Lawrence Livermore National on-14 isotope tracing with accelerator mass spectrometry lar-structure effects on soot formation in diesel engines.

2001-2003 New laboratories for homogeneous charge compression ignition (HCCI) engine research begin operation. Initial research identifies main source of CO emissions for HCCI engines and demonstrates how low-load combustion efficiency can be improved through charge stratification.





2002 CRF researchers demonstrate that soot formation in a diesel fuel jet can be avoided with the use of micro-orifices. The possibility of low NO_x and zero soot emissions is also demonstrated using EGR or low gas temperatures coupled with small orifices.

2003-2004 Detailed new understanding of the critical role in combustion and soot emissions played by interactions between fuel-jets, swirl, squish, and bowl design in high-speed diesels is developed. Results provide physical insight to guide the development of engine combustion systems and identify turbulence model requirements for engine computational fluid dynamics codes.

2004 Research on direct-injection (DI), hydrogen-fueled, spark-ignition engines initiated. Hydrogen-fueled DI engines offer the potential for diesel-like efficiency with ultra-low emissions. Research focuses on understanding hydrogen DI mixing processes.

A CRF-led team demonstrates the feasibility of laser-induced incandescence measurements of "real-world" particulate emissions on board a vehicle under actual driving conditions.

CRF coordinates a new research partnership and holds first working group meeting. The partnership, which involves ten automotive and heavy-duty engine manufacturers and five national laboratories, focuses on developing the science-base regarding clean, low-temperature (e.g., HCCI), advanced diesel combustion processes needed to develop the next generation of efficient, emission-compliant engines.

Atomic Oxygen

(Continued from page 1)

LIF detection of combustion-generated atomic oxygen. This photolytic interference is produced by single-photon dissociation of a precursor, whereas the LIF signal generation involves two-photon absorption. The different laser-intensity dependences of these processes suggest that excitation with a ps laser could be advantageous. To produce the same LIF signal, ps excitation requires significantly less laser energy than does ns excitation. Because photolytic production of O atoms increases as laser energy increases, ps excitation generates less interference from single-photon photolysis.

The advantage of ps excitation is evident from O-atom LIF line imaging in laminar premixed Bunsen flames. Figure 1 compares the ps LIF signal due to combustion-generated O atoms (labeled "ps-only LIF") to the signals resulting from O atoms that were photolytically produced using nonresonant ns laser pulses (labeled with the ns pulse energy). The ps pulse energy was sufficiently low to ensure that it caused negligible photodissociation. As shown in Figure 1, the interference from photolytically produced O atoms can overwhelm the signal from native O atoms in the flame

Flow flame interactions

The researchers also demonstrated the capability of two-dimensional O-atom LIF measurements of a flow-flame interaction. Measurements of transient flow-flame interactions are fundamental to understanding turbulent combustion. Repeatable flow-flame interactions provide well-controlled systems in which the effects of flow transients are studied.

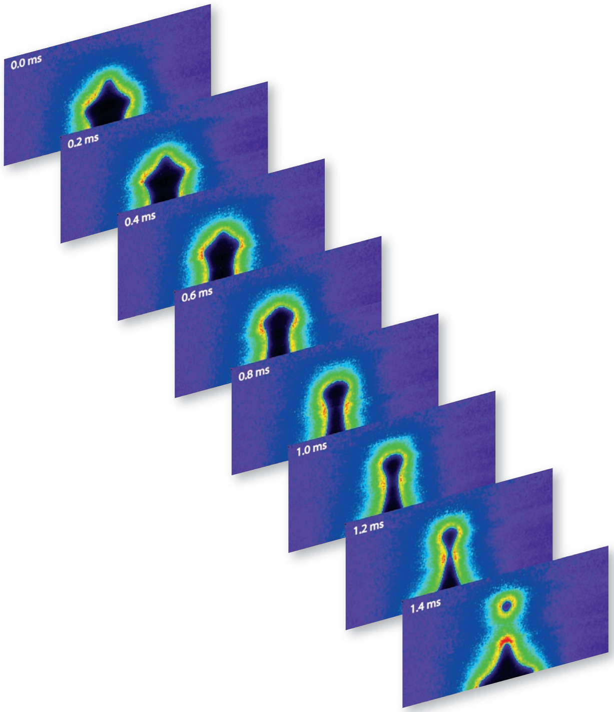


Figure 2. Temporal evolution of atomic oxygen in an acoustically forced axisymmetric premixed $CH_4/O_2/N_2$ flame. Each frame in the sequence is separated by 200 µs.

In Figure 2, the image sequence, which displays the temporal evolution of atomic oxygen in an acoustically forced Bunsen flame, demonstrates the ability to perform interference-free two-dimensional O-atom LIF measurements of a flow-flame interaction. The images show localized variations in O-atom levels that may result in locally increased thermal NO production. Measurements such as these could provide insight into the effects of transient flow-flame interactions on NO production.

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